Supplementary material for the article:

Anđelković, K.; Milenković, M. R.; Pevec, A.; Turel, I.; Matić, I. Z.; Vujčić, M.; Sladić, D.; Radanović, D.; Brađan, G.; Belošević, S.; et al. Synthesis, Characterization and Crystal Structures of Two Pentagonal-Bipyramidal Fe(III) Complexes with Dihydrazone of 2,6-Diacetylpyridine and Girard's T Reagent. Anticancer Properties of Various Metal Complexes of the Same Ligand. *Journal of Inorganic Biochemistry* **2017**, *174*, 137–149. https://doi.org/10.1016/j.jinorgbio.2017.06.011

Supplementary Information

Synthesis, characterization and crystal structures of two pentagonal-bipyramidal Fe(III) complexes with dihydrazone of 2,6-diacetylpyridine and Girard's T reagent. Anticancer properties of various metal complexes of the same ligand.

Katarina Anđelković,[a] Milica R. Milenković,[a] Andrej Pevec,[b] Iztok Turel,[b] Ivana Z. Matić,[c] Miroslava Vujčić,[d] Dušan Sladić,[a] Dušanka Radanović,[d] Gabrijela Brađan,[a] Svetlana Belošević,[e] Božidar Čobeljić[a1]

[a] *Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia*

[b] *Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia*

[c] *Institute of Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Republic of Serbia*

[d] *Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, P.O. Box 815, 11000 Belgrade, Serbia*

[e] *Faculty of Technical Sciences, University of Priština, Knjaza Milosa 7, Kosovska Mitrovica, Serbia*

Content:

Table S1. Crystal data and structure refinement details for **7** and **8**.

Table S2. Selected bond lengths (Å) and angles (°) for **7** and **8**.

[1]e-mail: bozidar@chem.bg.ac.rs

Table S1. Crystal data and structure refinement details for **7** and **8**.

	7	**8**
formula	$C_{22}H_{35}FeN_{10}O_4S_3$	$C_{47}H_{72}Fe_3N_{23}O_9S_9$
Fw (g mol^{-1})	655.63	1559.36
crystal size (mm)	0.40 × 0.02 × 0.02	0.15 × 0.10 × 0.05
crystal color	green	green
crystal system	triclinic	triclinic
space group	*P*–1	*P*–1
a (Å)	7.5016(9)	12.1021(3)
b (Å)	11.8462(10)	15.9085(5)
c (Å)	18.2010(15)	20.0448(6)
α (º)	82.959(7)	95.611(2)
β (º)	89.790(8)	95.470(2)
γ (º)	79.031(9)	110.266(3)
V (Å^3)	1575.6(3)	3568.24(19)
Z	2	2
calcd density (g cm^{-3})	1.382	1.451
F(000)	686	1618
no. of collected reflns	14602	33057
no. of independent reflns	7234	16315
R_{int}	0.1371	0.0453
no. of reflns observed	2972	10061
no. parameters	381	896
$R[I > 2\sigma(I)]^a$	0.0696	0.0694
wR_2 (all data)^b	0.1476	0.1891

Goof , S^c	0.872	1.044
maximum/minimum residual electron density (e $Å^{-3}$)	+0.64/–0.83	+2.50/–0.92

[a] $R = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$.
[c] $S = \{\sum[(F_o^2 - F_c^2)^2]/(n/p)\}^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

Table S2. Selected bond lengths (Å) and angles (°) for **7** and **8**.

7			
Fe1–N3	2.193(4)	O1–Fe1–N3	71.37(14)
Fe1–N4	2.208(4)	O1–Fe1–N4	140.86(16)
Fe1–N5	2.199(4)	O1–Fe1–N5	149.71(15)
Fe1–N8	2.031(4)	O1–Fe1–N8	90.44(14)
Fe1–N9	2.049(4)	O1–Fe1–N9	91.86(15)
Fe1–O1	2.079(3)	O1–Fe1–O2	78.00(13)
Fe1–O2	2.061(3)	N8–Fe1–N9	176.71(17)
8			
Fe1–N3	2.181(4)	O1–Fe1–N3	71.81(14)
Fe1–N4	2.200(3)	O1–Fe1–N4	141.57(14)
Fe1–N5	2.199(4)	O1–Fe1–N5	148.46(13)
Fe1–N8	2.039(4)	O1–Fe1–N8	90.42(15)
Fe1–N9	2.025(4)	O1–Fe1–N9	91.52(15)
Fe1–O1	2.092(3)	O1–Fe1–O2	76.81(13)
Fe1–O2	2.086(3)	N8–Fe1–N9	176.70(17)
Fe2–N12	2.197(4)	O3–Fe2–N12	71.69(14)
Fe2–N13	2.206(4)	O3–Fe2–N13	141.58(14)
Fe2–N14	2.180(4)	O3–Fe2–N14	148.41(14)
Fe2–N17	2.016(4)	O3–Fe2–N17	89.21(16)
Fe2–N18	2.043(4)	O3–Fe2–N18	92.88(14)
Fe2–O3	2.090(3)	O3–Fe2–O4	77.00(13)
Fe2–O4	2.100(3)	N17–Fe2–N18	176.28(17)
Fe3–N19	2.056(4)	N19–Fe3–O1w	90.45(17)
Fe3–O1w	2.076(4)	N21–Fe3–O1w	174.88(14)